Quantum phases in an asymmetric double-well optical lattice

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- Simulations of many-body systems with atoms in optical lattices.
- We are interested in lattice geometries with asymmetric double-wells along one axis, and single wells along perpendicular axes.
- This gives us a more general and richer Hamiltonian.
- Importantly, the Hamiltonian includes tunneling energies beyond nearest neighbors.
- Interaction between atoms at different sites become quite important.
- By tuning the lattice parameters, the goal is to be able to select 2 and 3 particle states, such that there is no two-body interaction energy, but finite three-body interaction energy.



Motivation...(long term)





Saurabh Paul Quantum phases in an asymmetric double-well optical lattice

Optical lattice potential

• The mathematical form for the double-well potential along x is

$$V(x) = -V_0 \cos^2(k_L x) - V_1 \cos^2[2k_L(x+b)].$$

- k_L is the laser wave vector.
- b controls the lattice asymmetry or tilt.
- $k_L b = \pi/4$ gives an untilted symmetric lattice.
- V_1/V_0 controls the barrier height between the left(L) and right(R) wells within a double well.
- In addition, the single well potential along y and z is

$$V_{\perp}(y,z) = -V_2 \left\{ \cos^2(2k_L y) + \cos^2(2k_L z) \right\}.$$





- Tunneling energies $t \gg J > J_L \approx J_R > J_{LR} > J_{RL}$.
- Interested in $t \gg \Delta$, where Δ is the lattice tilt.



Tunneling Energies, first construct Wannier functions

- Local Wannier functions are numerically obtained as eigen states of the position operatox x̂.
- The local wannier functions obtained are purely real.



Tunneling energies using Wannier functions

• Tunneling energies t, J, J_L, J_R, J_{LR} and J_{RL} are then obtained using the constructed local Wannier functions.

• For instance, $t = \langle w_L | \hat{H} | w_R \rangle$.



Tight Binding(TB) and Numerical(N) results for band tunneling energies (up to nearest neighbor unit cell)

Two approximations for TB Hamiltonian:

- $TB^{(1)}$, involving only nearest-neighbor hoppings, t & J,
- $TB^{(2)}$, involving all relevant hoppings, $t, J, J_L, J_R, J_{LR} \& J_{RL}$. $TB^{(1)}$ highly inadequate! Next-nearest-neighbor tunneling a must!!

 10^{0} $TB^{(2)}$. $\alpha = 2$ $\alpha \rightarrow Band Index$ Band Tunneling / E_R N, $\alpha = 2$ $TB^{(1)}$. $\alpha = 1,2$ $TB^{(2)}$. $\alpha = 1$ N, $\alpha = 1$ 5 10 15 20 25 30 Quantum Lattice depth V_0/E_R

Interaction terms ... using Wannier functions

- Bose-Hubbard Hamiltonian with two body interactions.
- For instance, $U_{LLLL} = g \int d\vec{r} w_L(\vec{r})^4$.
- U_{LLLR} , U_{LLRR} , $J \& J_L$ can be of same order, hence important!



Superfluid(SF) to Mott transition...Decoupling approximation (Mean field)

- Write down a Bose Hubbard Hamiltonian
 - including all relevant hoppings, $t, J, J_L, J_R, J_{LR} \& J_{RL}$,
 - including all relevant interaction terms, U_{LLLL}, U_{RRRR} & U_{LLRR}.
- Ose the decoupling approximation

$$a_{i,L}^{\dagger}a_{j,R} = \psi_L a_{j,R} + \psi_R a_{i,L}^{\dagger} - \psi_L \psi_R,$$

- $a_{i,L}^{\dagger}, a_{j,R} \rightarrow$ creation, annihilation operators,
- $\psi_L = \langle a_L \rangle$ and $\psi_R = \langle a_R \rangle$,
- ψ_L & ψ_R are the site independent order parameters.
- So Minimize ground state energy $E_g(\psi_L, \psi_R)$ obtained using 2^{nd} order perturbation theory. Then, for $E_g^{min}(\psi_L, \psi_R)$, if
 - $\psi_L \& \psi_R = 0 \rightarrow \text{Mott state.}$
 - $\psi_L, \psi_R \neq 0 \rightarrow \text{Superfluid state.}$

Mott lobes

- Effective tunneling along x, $t_{eff} \approx t + J$.
- Mott lobes are 'chopped' at $t_{eff} pprox 4 J_{\perp}$.
- SF state for $t_{eff} \ge 4J_{\perp}$.



- Studied a general asymmetric double-well lattice.
- Discussed method to construct the local Wannier functions.
- Showed that an acceptable TB model must include next-nearest-neighbor hoppings.
- Showed that interactions beyond on-site terms are quite important.
- Obtained the phase diagram using decoupling approximation.
- Need to carefully choose states for zero two body and finite three body interactions.
- Need to devise suitable lattice transformations to make atoms populate such states.

